

Dipropylamine
142-84-7 | DTXSID2025185

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.75e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.83e-01

Confidence level: 6.94e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dipropylamine</div> <div>Measured: 5.79e-01</div> <div>Predicted: 7.75e-01</div>	<div>Image not found</div> <div>N-Ethyl-N-butylamine</div> <div>Measured: 3.63e-01</div> <div>Predicted: 7.00e-01</div>	<div>Image not found</div> <div>Diisopropylamine</div> <div>Measured: 1.09</div> <div>Predicted: 1.10</div>
<div>Image not found</div> <div>Triethylamine</div> <div>Measured: 7.28e-01</div> <div>Predicted: 7.20e-01</div>	<div>Image not found</div> <div>2-Propanamine, N-ethyl-</div> <div>Measured: 11.5</div> <div>Predicted: 5.69</div>	